Claims

1. A Method for sampling a state space by iteratively generating states $x_{i,t}$ and their weighting factors $\tilde{\rho}_{i,t}$, wherein the index i is the iteration parameter and the index t distinguishes different states $x_{i,t}$ generated by an iteration i, the method is consisting of
a first step for selecting an initial sampling distribution function $\rho_1(x)$,
a fifth step for performing an analysis
and an iteration procedure including
a second step for generating N_j states $x_{j,t}$ by a numerical sampling algorithm and
a fourth step for testing at least one criterion to decide whether to continue the iteration procedure or to stop the iteration procedure and to go to a fifth step in order to perform the analysis using the simulated data,
characterized in that the iteration procedure further includes
a third step determining weighting factors $\tilde{\rho}_{i,t}$ for states $x_{i,t}$ generated so far by using sampling distribution functions $\rho_i(x)$ determined so far and
a fitting step for determining a sampling distribution function $\rho_j(x)$ for the next iteration by fitting $\rho_j(x)$ to $\tilde{\rho}_{i,t}O(x_{i,t})$ for states $x_{i,t}$ generated so far, wherein $O(x_{i,t})$ is a function, respectively a property, of the states $x_{i,t}$.

2. Method as claimed in claim 1, wherein the sampling distribution function $\rho_j(x)$ of at least one iteration is fitted such that it maximises an objective function preferably defined as a function of local comparisons between the sampling distribution function and the product $\tilde{\rho}_{i,t}O(x_{i,t})$.

3. Method as claimed in claim 1 or 2, wherein the sampling distribution function $\rho_j(x)$ of at least one iteration is fitted such that the sampling distribution function $\rho_j(x)$ is large for at least one state $x_{i,t}$ with a large product $\tilde{\rho}_{i,t}O(x_{i,t})$, and tends to be small for states with a small product $\tilde{\rho}_{i,t}O(x_{i,t})$.

4. Method as claimed in one of claims 1 to 3, wherein the sampling distribution function $\rho_j(x)$ of at least one iteration is a function with at least one constraint, preferably having an extreme value in the region of at least one selected state $x_{j,constr}$ and having vanishing values at a distance from the at least one selected state $x_{j,constr}$, wherein the constraint is

preferably a harmonic constraint with at least one constant k_{constr} defining the strength of the constraint at the selected state $x_{j,constr}$.

5. Method as claimed in claim 4, wherein the sampling distribution function $\rho_j(x)$ of at least one iteration is the distribution function of the system with constraints or a multicanonical distribution function with constraints.

6. Method as claimed in claim 1 or 2, wherein the numerical sampling algorithm of at least one iteration generates correlated states $x_{j,t}$, wherein the sampling distribution function $\rho_j(x)$ preferably has a maximum that biases sampling into a sub-region of the state space, wherein the sampling distribution function $\rho_j(x)$ is preferably fitted such that the maximum is in a region where the product $\tilde{\rho}_{i,t}O(x_{i,t})$ has a maximum, and wherein the sampling preferably starts from a state close to the maximum of the sampling distribution function $\rho_j(x)$.

7. Method as claimed in one of claims 4 to 6, wherein the fitting of $\rho_j(x)$ is done by selecting states $x_{i,t}$ for which the product $\tilde{\rho}_{i,t}O(x_{i,t})$ has extreme values and by using the selected states $x_{i,t}$ to define the region in which $\rho_j(x)$ has extreme values.

8. Method as claimed in one of claims 1 to 6, wherein parameters of the sampling distribution function $\rho_j(x)$ of at least one iteration are determined by a linear least square fit of the logarithm of the un-normalized sampling distribution function $\rho_j(x)$ to the logarithm of the product $\tilde{\rho}_{i,t}O(x_{i,t})$

9. Method as claimed in one of claims 1 to 8, wherein the normalization constant of the sampling distribution function $\rho_j(x)$ of at least one iteration is estimated from the sampled states $x_{i,t}$ and their weighting factors $\tilde{\rho}_{i,t}$.

10. Method as claimed in one of claims 1 to 9, wherein at least three iterations are done.

11. Method as claimed in one of claims 1 to 10, wherein the function $O(x)$ is a function of a set of at least two functions $\Theta=\{O_1(x),O_2(x),\ldots,O_{N_{prop}}(x)\}$, preferably including at least one of the following functions

at least one property for which at least one estimate is derived in the analysis of the fifth step,

at least one function that is large for states that must be sampled to ensure transitions between important regions,

the inverse of the probability distribution function of at least one property of the system, and

the inverse of the probability distribution of the negative logarithm of the distribution function of the system .

12. A computer software product for sampling a state space by iteratively generating states $x_{i,t}$ and their weighting factors $\tilde{p}_{i,t}$, wherein the index i is the iteration parameter and the index t distinguishes different states $x_{i,t}$ generated by an iteration i, said product is characterized by a computer-readable medium in which program instructions are stored, which instructions, when read by a computer, enable the computer to

select an initial sampling distribution function $\rho_1(x)$,

to execute a fifth step for performing an analysis

and to execute an iteration procedure including

a second step for generating N_j states $x_{j,t}$ by a numerical sampling algorithm and

a fourth step for testing at least one criterion to decide whether to continue the iteration procedure or to stop the iteration procedure and to go to a fifth step in order to perform the analysis using the simulated data,

characterized in that the iteration further includes

a third step determining weighting factors $\tilde{p}_{i,t}$ for states $x_{i,t}$ generated so far by using sampling distribution functions $\rho_i(x)$ determined so far and

a fitting step for determining a sampling distribution function $\rho_j(x)$ for the next iteration by fitting $\rho_j(x)$ to $\tilde{p}_{i,t}O(x_{i,t})$ for states $x_{i,t}$ generated so far, wherein $O(x_{i,t})$ is a function, respectively a property, of the states $x_{i,t}$.